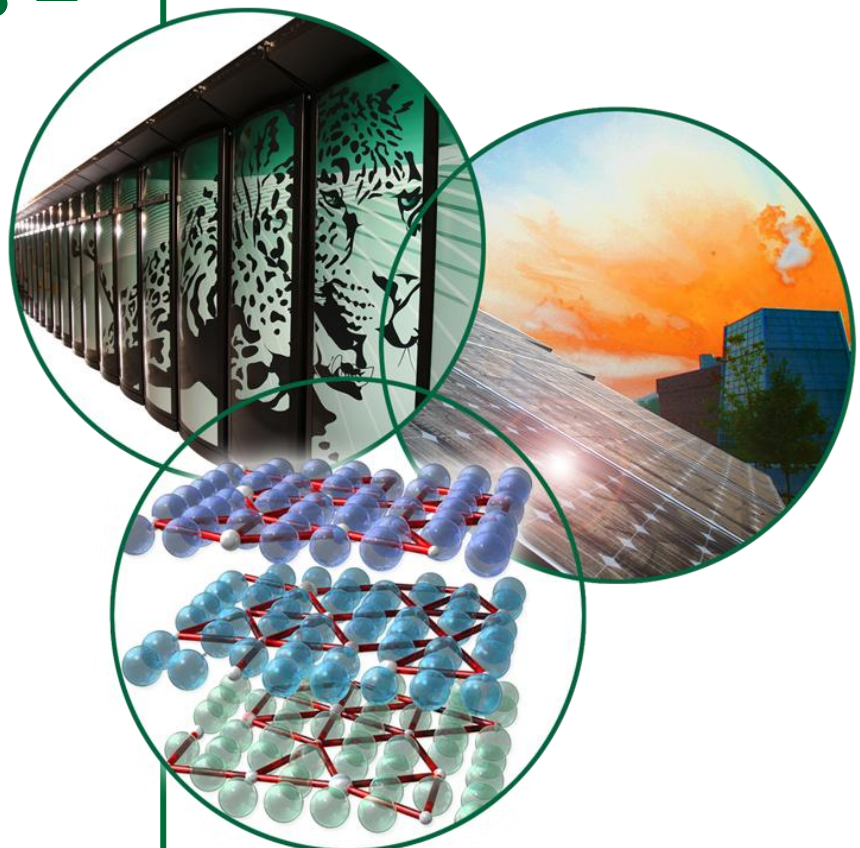
ORIGEN Isotopic Depletion Capabilities – Overview and Status Update

Nuclear Physics Working Group Meeting
Brookhaven National Laboratory
2009 November 6



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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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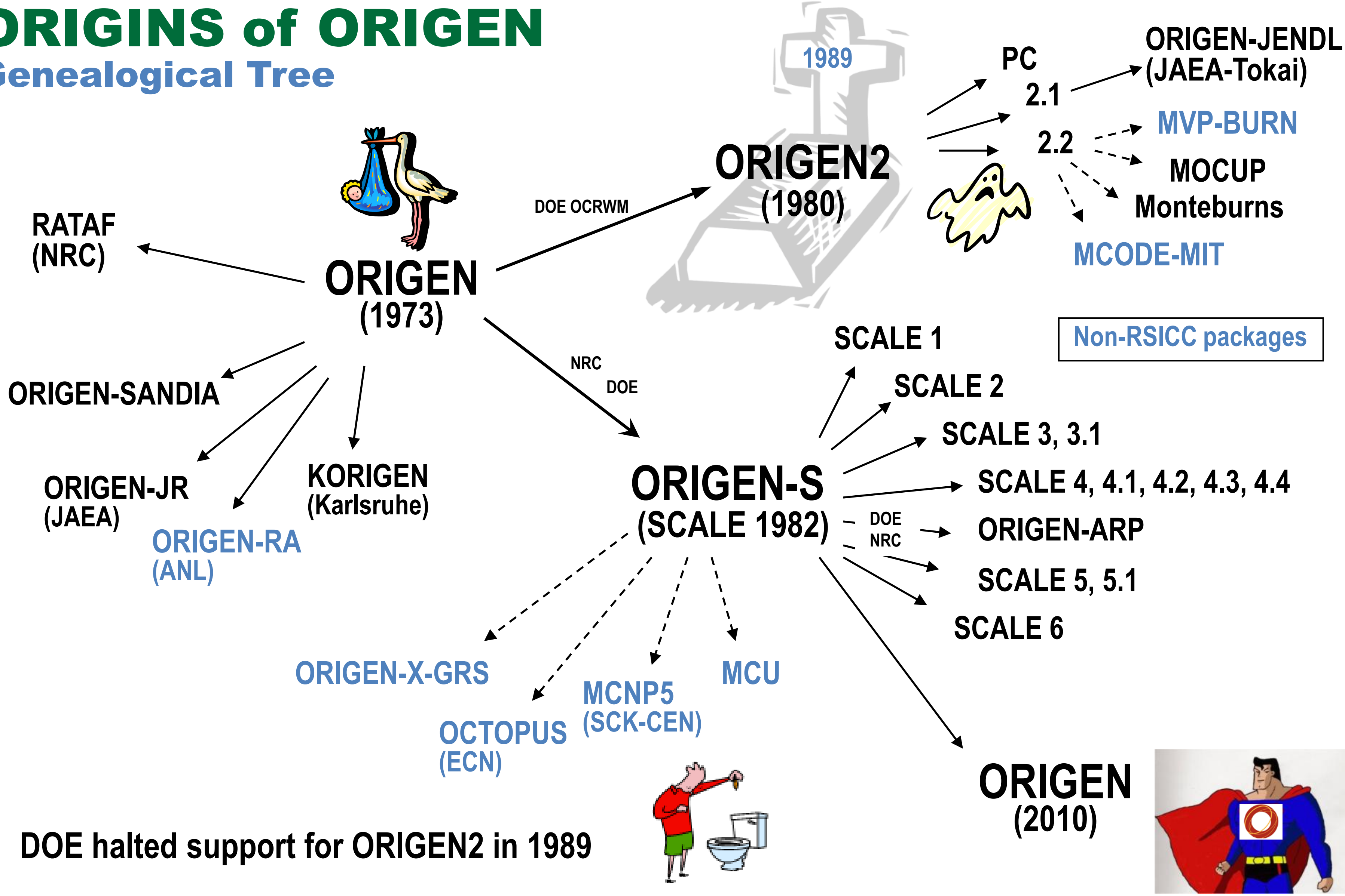
Content

- Origins of ORIGEN
  - Modeling and simulation capabilities
  - Development history, status, versions
  - SCALE – current state-of-the-art ORIGEN capability and data
- Code/data requirements for physics applications
  - Nuclear data for isotopic transmutation
  - Neutron and gamma radiation source terms
- Validation database

ORIGEN – Oak Ridge Isotope Generation and Decay Code

- Irradiation and decay, batch and continuous chemical processing
- ORIGEN is a coupled differential equation solver
  - Designed for difficult problems involving extremely diverse rate constants
- Code calculates:
  - Time dependent isotopic concentrations and radioactivity
  - Decay heat (based on summation)
  - Radiation sources (neutron/gamma)
  - Radiotoxicity
- Massive nuclear database for all nuclides produced by neutron transmutation, fission, and activation: 2227
  - 904 activation nuclides
  - 174 actinides
  - 1149 fission products
  - Complete data enable code to characterize irradiated fuel and components from seconds to millions of years after irradiation
- If you have been involved in fuel cycle or spent fuel analysis, you have probably used ORIGEN or seen it used
  - Thousands of licensed users: SCALE 5.1=1600, SCALE 6 (>500 in first 6 months)
  - Used worldwide; in every continent (except Antarctica)

ORIGINS of ORIGEN
Genealogical Tree



- DOE halted support for ORIGEN2 in 1989
- DOE and NRC continue to support development of ORIGEN in SCALE

Use and Misuse of ORIGEN2

- Widespread cavalier use of ORIGEN2 reactor libraries beyond designed range of application with serious consequences in analysis results
  - Nuclear data was developed for plant operations and fuel types in 1980s
  - Cross section and decay data are obsolete
  - No high burnup capability
  - No high enrichment capability
  - Limited MOX capability, no advanced reactors, no research reactors
  - Dated neutron and gamma ray source capability
  - Limited published studies involving isotopic validation (data representation lacks the necessary fidelity for problem dependent application)

  - But… it is designed for standalone analysis and is easy to use

- Unless you have completely regenerated the nuclear data in ORIGEN2, you should not be using this code

Nuclear Data Needs for Fuel Cycle Applications

- Broad range of fuel cycle applications requires powerful and adaptable codes and state-of-the-art nuclear data
- Data must adapt to the application physics
  - Thermal and fast reactor fuel analysis
  - High burnup fuel
  - Material activation and nuclear forensics
  - Nuclear safeguards and non-proliferation (passive NDA and active interrogation)
  - Waste management
- Application area data requirements
  - Higher actinide transmutation (Am, Cm, Cf) required accurate modern cross sections
  - Attribution and forensics - Expanded number of reaction types for production of low concentration signatures
  - Comprehensive gamma ray library (NDA)
  - Accurate neutron source methods and data (inherent neutron source and sources used for neutron interrogation of SNM)

ORIGEN – Data for the Next Generation

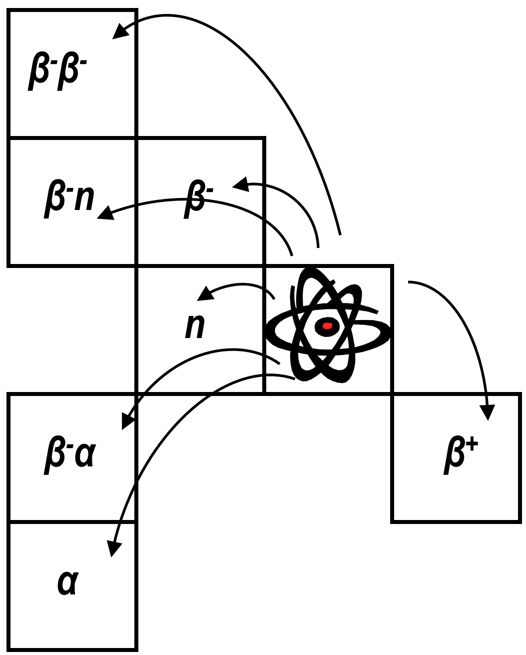
- ORIGEN contains a massive collection of nuclear data
  - 2600 decay transitions
  - Approx. 16,000 neutron-induced reaction transitions (byproducts)
  - Approx. 34,000 fission production yield transitions
- Explicit simulation of all decay and reaction pathways
  - ORIGEN accurately represents of the evaluated nuclear data
  - No approximations
- In ORIGEN, all problem dependent data are calculated dynamically
  - 774 nuclide cross sections recalculated at each time point
  - Fission yields adjusted to the fission spectrum for each actinide
  - Neutron branching fractions recalculated
- Data developed from ENDF/B evaluations
  - Cross Sections (MF3, MF10)
  - Multiplicity – branching fractions (MF3+MF9)
  - Direct fission yields (MF8, MT454)
    - Thermal (0.0253 eV)
    - Fast (500 keV) – Pooled measurements from 500 keV to 2 MeV
    - High energy (14 MeV)

ORIGEN Nuclear Database

- **ENDF/B-VII decay data**
- **Cross Sections from JEFF-3.1/A** http://www.nea.fr/html/dbdata/JEFF/JEFF31/JEFF-3A.pdf
  - **Special purpose activation cross section evaluations (< 20 MeV)**
  - **774 target nuclei, 12,617 neutron-induced reactions**
  - **JEFF-3.1/A developed from continuous-energy EAF-2003 evaluations in standardized ENDF format**
  - **Processed to multigroup format (44-, 47-, 199-, 200-, and 238-groups)**
  - **Includes cross sections for > 20 different reaction types**
    - **Other ORIGEN and ORIGEN2 variants limited to (n,g), (n,p), (n,f), (n,α), (n,2n), (n,3n)**
  - **Reactions to isomer states handled as partial cross section – method implicitly treats energy-dependent branching to excited states**
  - **All reaction byproduct generation included**
- **Energy-dependent ENDF/B-VII fission yields**

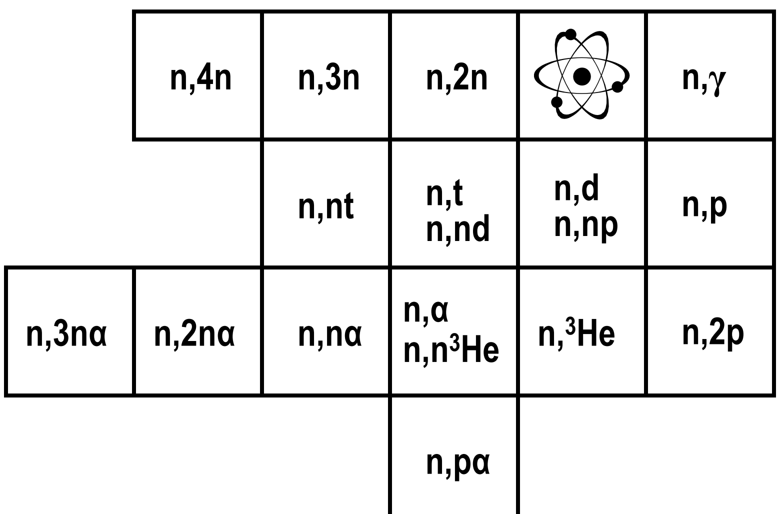
Nuclear Decay Data

- Upgraded to ENDF/B-VII
  - β^-, β^+, EC, α, IT, $\beta^-\beta^-$, β^-n, n, $\beta^-\alpha$
  - Transitions to ground and excited states



Nuclear Cross Section Data

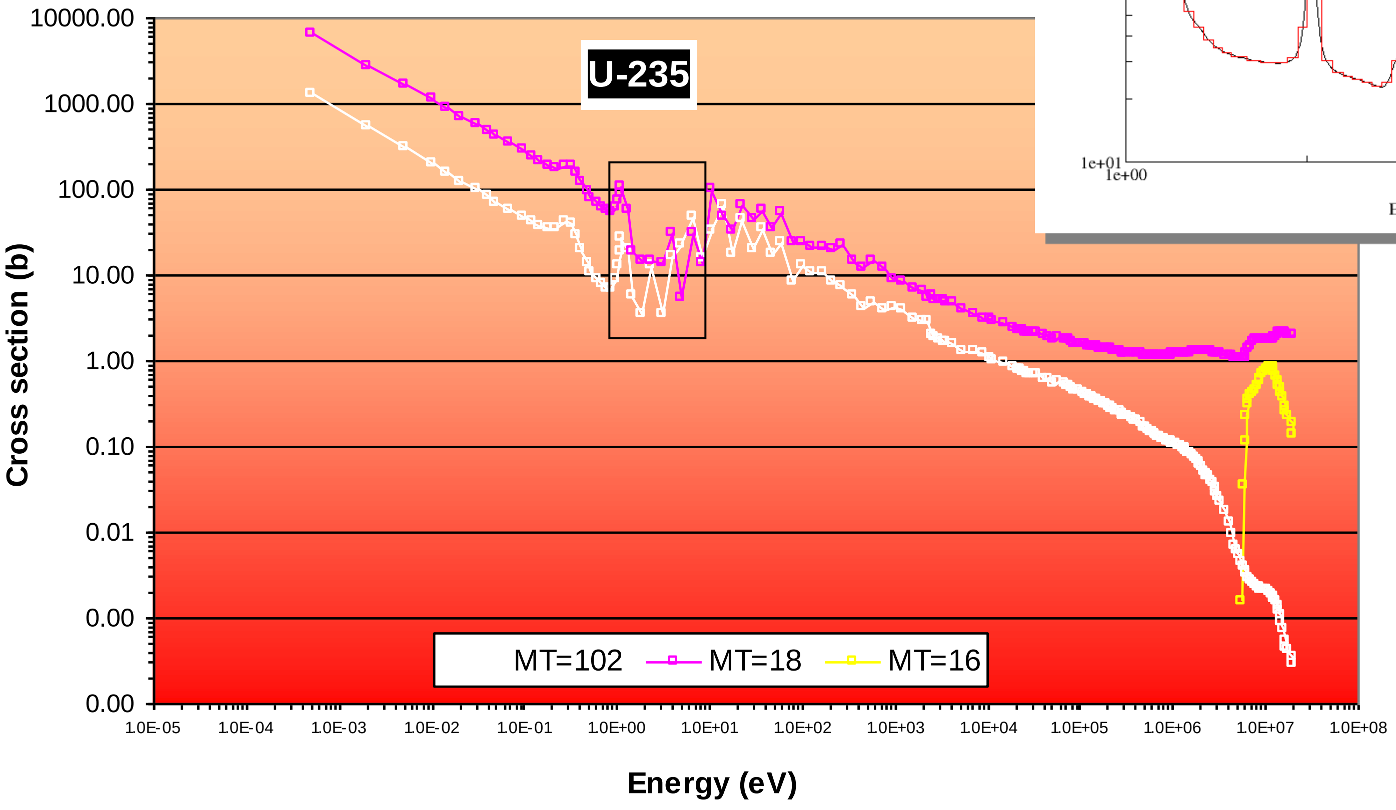
- JEFF-3.1/A + ENDF/B-VII data
  - Reaction types supported (n,2n), (n,3n), (n,f), (n,nα), (n,n3α), (n,2nα), (n,3n α), (n,np), (n,n2α), (n,2n2α), (n,nd), (n,nt), (n,n ^{3}He), (n,nd2α), (n,nt2α), (n,4n), (n,g), (n,p), (n,d), (n,t), (n,^{3}He), (n,α), (n,2α), (n,3α), (n,2p), (n,pα), (n,t2α), (n,d2α), (n,n')
  - Transitions to ground and excited states + n,n' (MT51)
  - General transition matrix formed for nuclide A → B
  - Solver methods allow cyclic feedback A ⇆ B

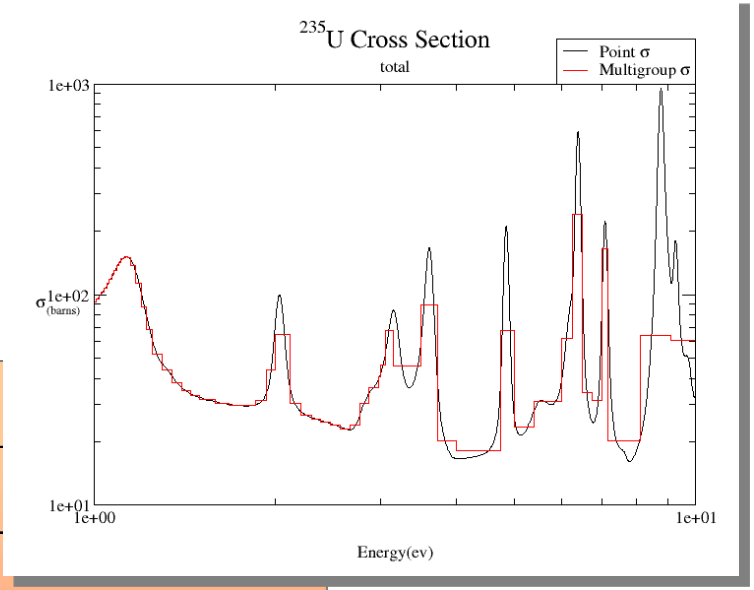


Reaction Type	Number of reactions in JEFF-3.1/A library
(n,n')	262
(n,2n)	1010
(n,3n)	871
(n,f)	90
(n,n'α)	907
(n,2nα)	4
(n,3nα)	2
(n,n'p)	922
(n,n2α)	1
(n,n'd)	904
(n,n't)	791
(n,n'h)	208
(n,4n)	25
(n,2np)	7
(n,γ)	1007
(n,p)	1016
(n,d)	927
(n,t)	951
(n,h)	862
(n,α)	992
(n,2α)	2
(n,2p)	822
(n,pα)	34

ORIGEN Cross Sections (MF3,MF10)

JEFF-3.1/A 200 neutron groups





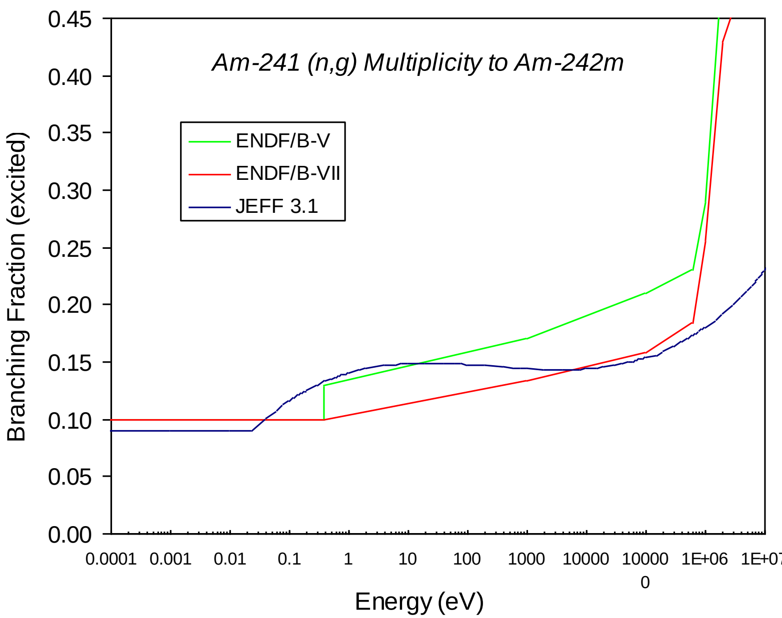
Multiplicity (MF9)
Branching leading to production of an isomeric state

- Energy dependence now calculated dynamically
  - ORIGEN uses energy-dependent cross sections to each product state
- <u>Most codes assume isomeric branching is a constant value</u>
- Example: ^{241}Am (n,γ) $\xrightarrow{f\gamma'}$ ^{242m}Am (n,γ) $T_{1/2}$= 114 y
  $\rightarrow$ ^{242}Am (n,γ) $T_{1/2}$= 16 h

thermal fγ' values

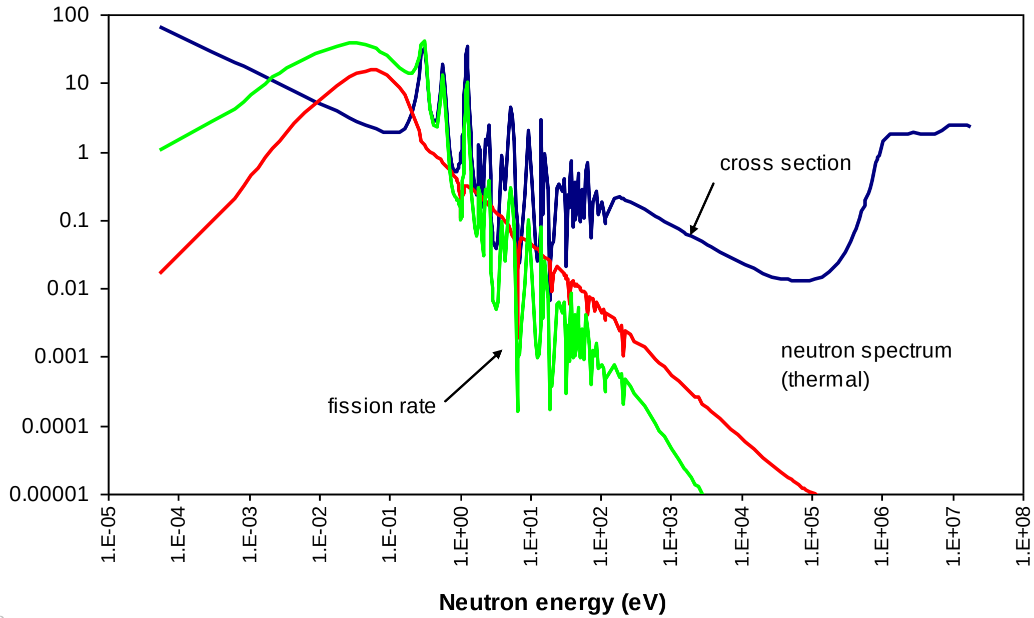
ORIGEN-S*	16.2%
IAEA WIMS	12.0%
ORIGEN2	20.0%
ENDF/B-VII	10.0%
JEFF 3.1	9.0%

* Previous releases
Recommended value based on detailed evaluation of destructive measurements 11%



Fission Yields (MF8,MT454)

- Independent fission yields calculated using energy-dependent fission spectrum for each actinide
- 1149 fission products
- 30 fissionable actinides
- Fraction of fissions occurring in each energy region of tabulated ENDF/B-VII yields used to weight effective fission yield



Photon Yield Library

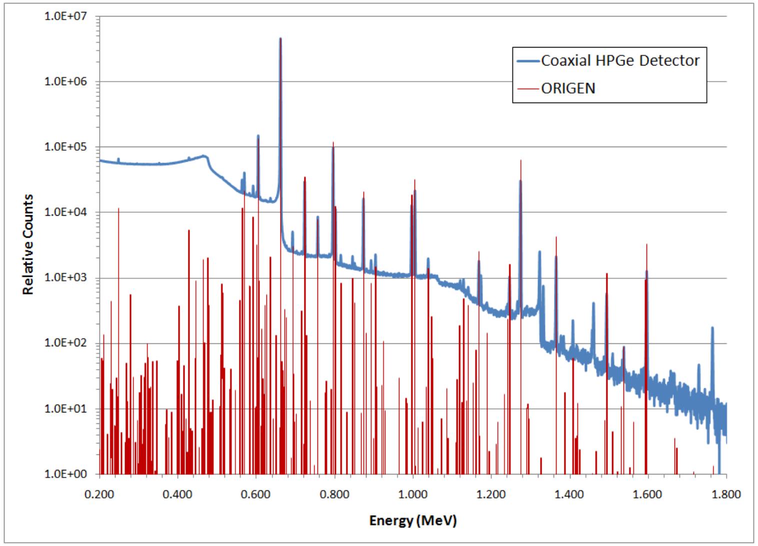
- Library of gamma ray intensity and yield for all evaluated radioactive isotopes
  - 1132 gamma emitting nuclides (ENDF/B-VI, ENSDF, JEFF)
- Discrete gamma lines due to
  - β-, β+, α, IT, ε decay
- Discrete X-rays due to
  - β+ annihilation radiation
  - Fluorescence following K-capture (ε) or emission of conversion electrons
- Continuum gamma spectra due to
  - Theoretical spectra based on nuclear structure calculations
- Continuum X-ray spectra due to
  - Internal Bremsstrahlung processes

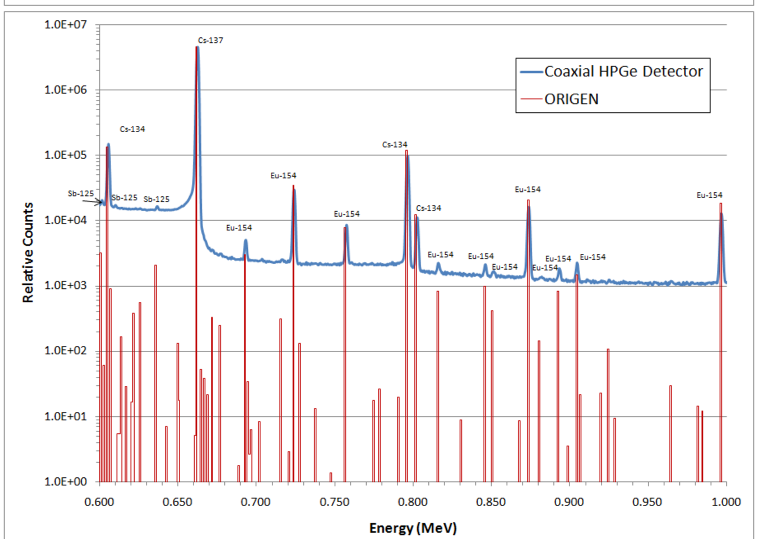
- Earlier version (ORIGEN2) library developed in 1979 with 418 radionuclides
  - Missing many short-lived fission products
  - Missing many key activation and medical isotopes

Gamma Analysis Applications

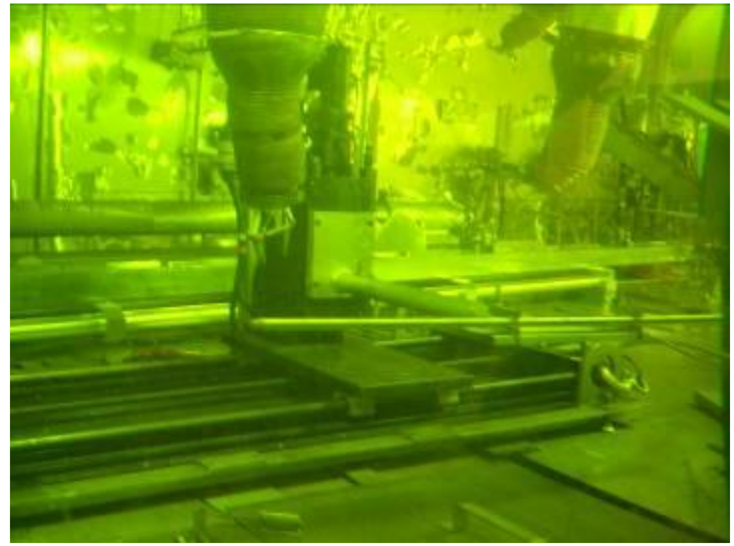
Spent nuclear fuel non-destructive analysis

Spent Fuel Gamma Spectra (TMI-1)

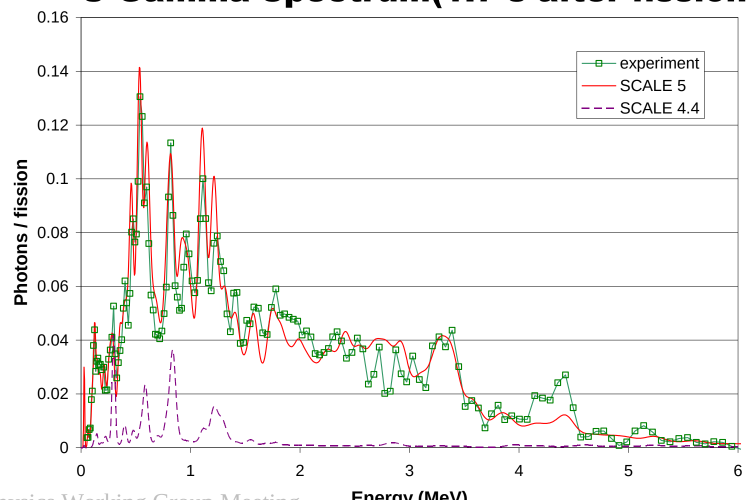




Fuel examinations

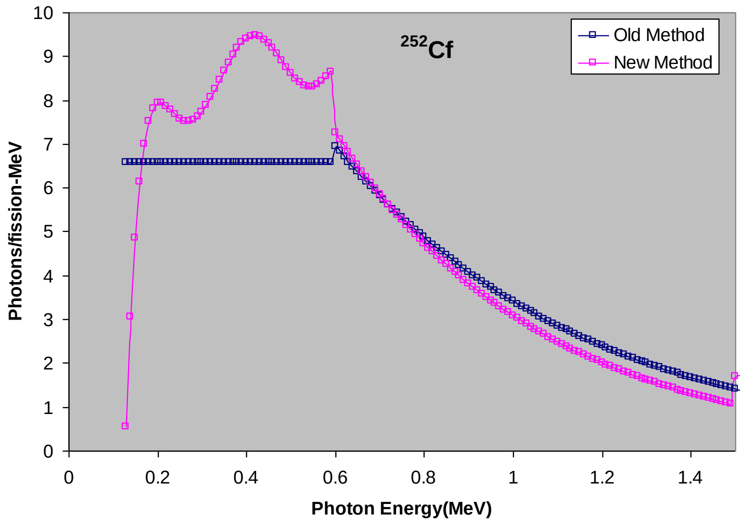


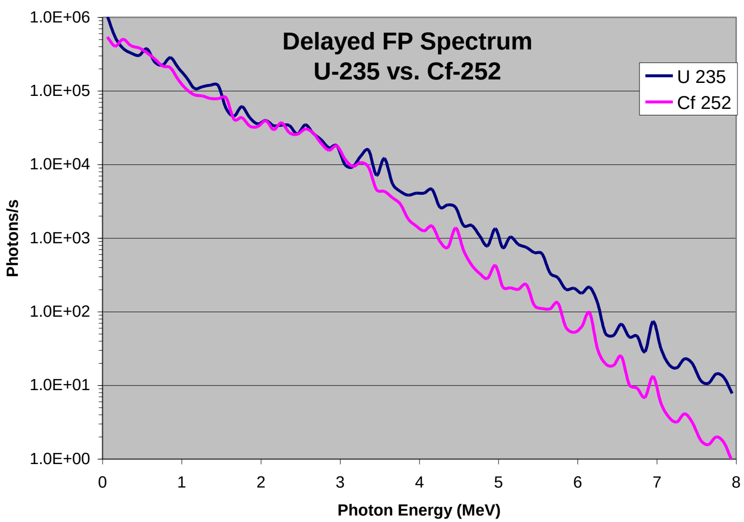
^{235}U Gamma Spectrum(1.7 s after fission)



Spontaneous Fission Gamma Rays

- Work recently done with Georgia Tech on ^{252}Cf source analysis
- Prompt-only gamma spectrum implemented
- Time dependent fission products simulated explicitly using ENDF/B-VII spontaneous fission yields
  - Delayed fission product gamma rays represent ~50% of the total emission rate





Neutron Source Methods

- Methods based on LANL SOURCES-4C code homogeneous option
  - Gauld, Shores, Perry - http://www.ornl.gov/~webworks/cppr/y2001/pres/113058.pdf
  - Spontaneous fission: Watt fission spectrum parameters for 41 actinides
    - $N(E) = C\, e^{-E/A} \sinh (B\, E)^{1/2}$
    - ν values and SF branching fractions
  - (α,n) reaction neutrons
    - Stopping power method $$Y_i = \frac{N_i}{N} \int_0^{E_\alpha} \frac{\sigma_i(E)}{S(E)} dE$$
    - 89 α-emitting actinides and 7 α-emitting fission products
    - 19 light target nuclides: ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O, ^{19}F, ^{21}Ne, ^{22}Ne, ^{23}Na, ^{25}Mg, ^{26}Mg, ^{27}Al, ^{29}Si, ^{30}Si, ^{31}P, and ^{37}Cl
  - Delayed neutron spectra for 105 fission products – spectra in 10 keV bins starting at 50 keV as in ENDF/B

Inverse Problems and Adjoint Solutions

- ORNL has developed an Adjoint version of ORIGEN for inverse problems
- Automatic differentiation also applied successfully using GRESS (Gradient Enhanced Software System); OpenAD (Argonne)
  - I. C. Gauld and D. E. Mueller, "Evaluation of Cross-Section Sensitivities in Computing Burnup Credit Fission Product Concentrations," ORNL/TM-2005/48 (2005).
- INDEPTH Software for automated parameter search with least squares optimization
  - C. F. Weber and B. L. Broadhead, "Inverse Depletion/Decay Analysis Using the SCALE Code System," *Trans. Am. Nucl. Soc.*, 95, 248–249 (2006).
  - Nuclear Forensic applications – Spent Nuclear Fuel

Reactor (Assembly)	Burnup (GWd/MTU)		Decay time (d)		Enrichment (%)	
	Actual	Predicted	Actual	Predicted	Actual	Predicted
Calvert Cliffs (BT03)	46.5	43.5	2447	2832	2.45	2.30
Gosgen (GU3)	52.4	53.0	NA	1332	4.10	4.27
Mihama-3 (87C03)	31.4	28.7	1825	1863	3.24	3.21
Trino (ESL7)	24.5	26.2	NA	584	3.13	3.35
Turkey Point (D04/RG10)	31.3	30.3	927	1273	2.56	2.52
Takahama (SF96-4)	28.9	29.5	0	15.6	2.63	2.90
Takahama (SF97-4)	47.0	46.8	0	1	4.11	4.16

Application V&V

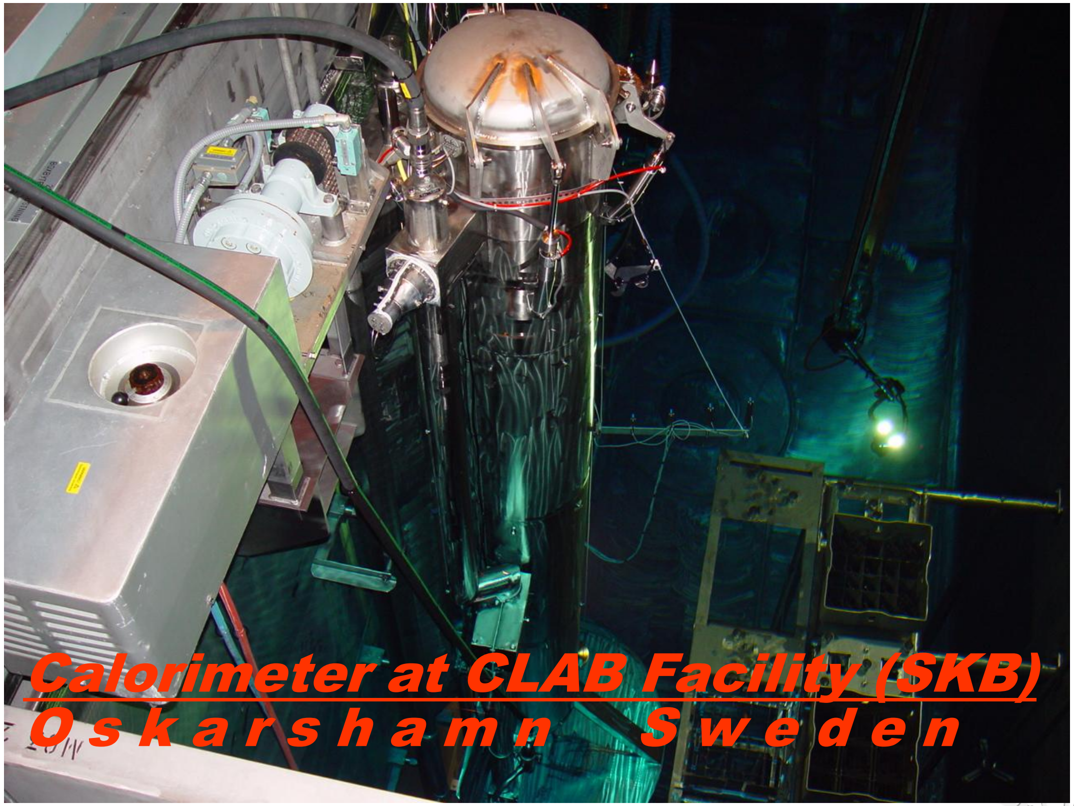
- ORNL has a longstanding commitment to ORIGEN V&V
- ORNL has provided guidance to DOE and NRC on data acquisition and worked to acquire and evaluate data from U.S. and international programs
  - Isotopic benchmark measurements for more than 160 spent fuel samples, including
    - OECD/NEA SFCOMPO database http://www.nea.fr/sfcompo/
    - TMI-1 measurements
    - ARIANE, REBUS, and MALIBU high burnup International programs
    - High burnup Spanish PWR fuel measurements (75 GWd/t)
    - New modern BWR data being acquired for Sweden
- Decay heat measurements
  - More than 100 assemblies measured in Sweden circa 2006
  - Short cooling times < 5 hours after fission
- Neutron and gamma ray delayed emission spectra

ORIGEN Spent Fuel Isotopic Validation Sets

Reactor (country)	Measurement facility	Experimental program	Assembly design	Enrichment (wt % ^{235}U)	No. of samples	Burnup (GWd/t)
TMI-1 (USA)	ANL (USA)	OCRWM YMP	15 × 15	4.013	11	44.8 – 55.7
TMI-1 (USA)	GE-VNC (USA)	OCRWM YMP	15 × 15	4.657	8	22.8 – 29.9
Calvert Cliffs (USA)	PNNL, KRI (USA, Russia)	OCRWM ATM	14 × 14	2.5 / 2.7 3.0	9	18.4 – 44.3
Takahama 3 (Japan)	JAEA (Japan)	JAEA	17 × 17	2.63 / 4.11	16	14.3 – 47.3
Obrigheim (Germany)	ITU/IAEA/WAC/IRCh (Germany)	JRC	14 × 14	3.8 / 3.13	28	15.6 – 38.1
Trino Vercellese (Italy)	Karlsruhe (Germany)	JRC	15 × 15	2.7 / 3.1 / 3.9	31	7.2 – 25.3
H.B. Robinson Unit 2 (USA)	PNNL (USA)	OCRWM ATM	15 × 15	2.56	4	16.0 – 31.6
Turkey Point (USA)	Battelle Columbus (USA)	NWTS	15 × 15	2.56	5	30.5 – 31.6
Gosgen (Switzerland)	SCK-CEN, ITU (Belgium, Germany)	ARIANE	15 × 15	4.1	3	29.1 / 52.5 / 59.7
GKN II (Germany)	SCK-CEN (Belgium)	REBUS	18 × 18	3.8	1	54.0
Vandellós II (Spain)	Studsvik Nuclear (Sweden)	CSN/ENUSA	17 × 17	4.498	7	42.9 – 73.8
Gösgen (Switzerland)	SCK-CEN (Belgium)	MALIBU	15 × 15	4.3	3	46.0 / 50.8 / 70.4

ORIGEN Decay Heat Validation
Swedish spent fuel measurements

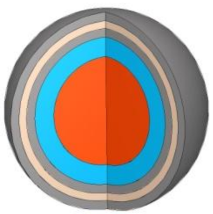
- High burnup fuel data
- Extended cooling times < 30 years
- Modern fuel assembly designs



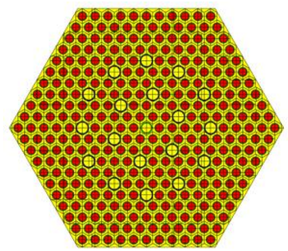
SCALE Depletion Capabilities

Standardized Computer Analysis for Licensing Evaluation

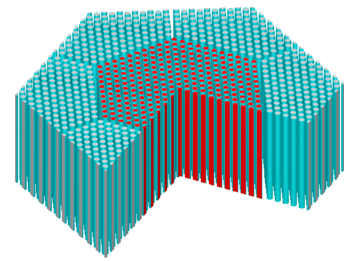
- **TRITON depletion sequence performs 1-D, 2-D, or 3-D analysis**



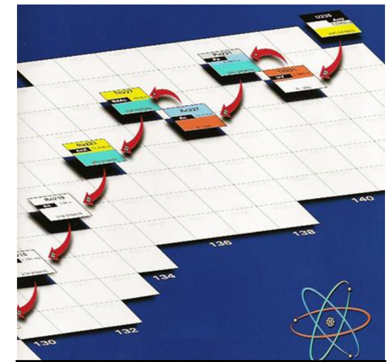
XSDRNPM – 1-D SN (SCALE 6.1)



NEWT – 2-D SN



KENO-V (-VI) – 3-D MC



ORIGEN Libraries

  - **Couples transport code with depletion/decay code ORIGEN-S**
  - **Rigorous treatment of the resonance self-shielding using the CENTRM/PMC methodology**
    - **problem-dependent pointwise energy flux (50,000-70,000 energy points) from 1-D transport calculation with CENTRM for system components**
    - **CENTRM flux solution used by PMC to collapse the pointwise cross section data to obtain problem-dependent multigroup cross sections (238-group) for transport calculations**

Distributed Reactor and Assembly Libraries

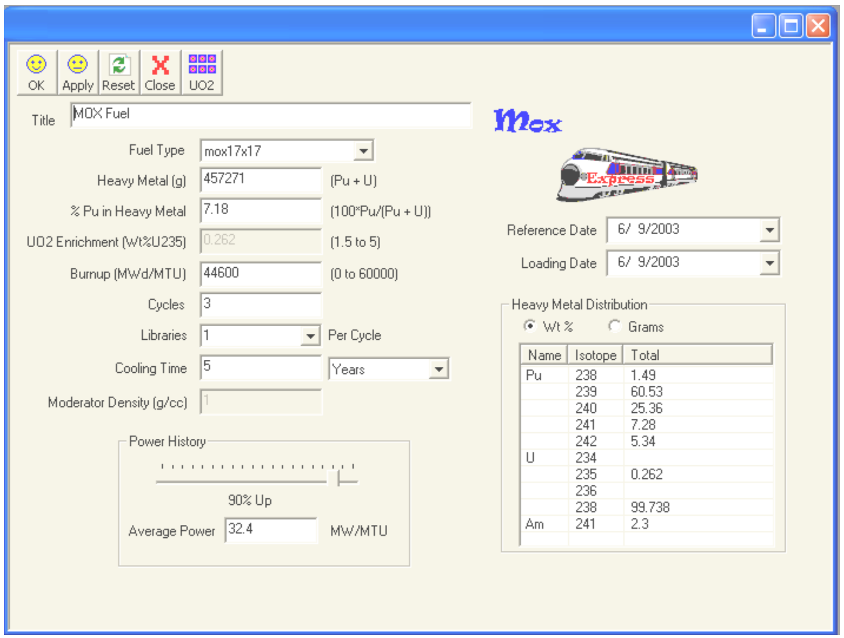
Reactor Type*	Assembly Design Description
PWR LEU* 1.5 – 6.0 wt% 72 GWd/t	Combustion Engineering 14x14
	Combustion Engineering 16x16
	Westinghouse 14x14
	Siemens 14x14
	Westinghouse 15x15
	Westinghouse 17x17
	Westinghouse 17x17 OFA
BWR LEU* 1.5 – 6.0 wt% 72 GWd/t	GE 7x7
	GE 8x8
	ABB 8x8
	GE 9x9
	GE 10x10
	ATRIUM-9 9x9
	ATRIUM-10 10x10
	SVEA-64 8x8
	SVEA-100 10x10

VVER LEU	VVER-440 1.6%, 2.4%, 3.6%
	VVER-440 3.82%
	VVER-440 4.25%
	VVER-440 4.38%
	VVER-1000
CANDU	CANDU 37 element natural uranium
	CANDU 28 element natural uranium
MAGNOX	Natural uranium
AGR	LEU
RBMK	1.8 – 2.2 wt%
PWR MOX	14x14
	15x15
	16x16
	17x17
	18x18
BWR MOX	8x8-2
	9x9-1
	9x9 ATRIUM-9
	10x10 ATRIUM-10

Visualization Tools

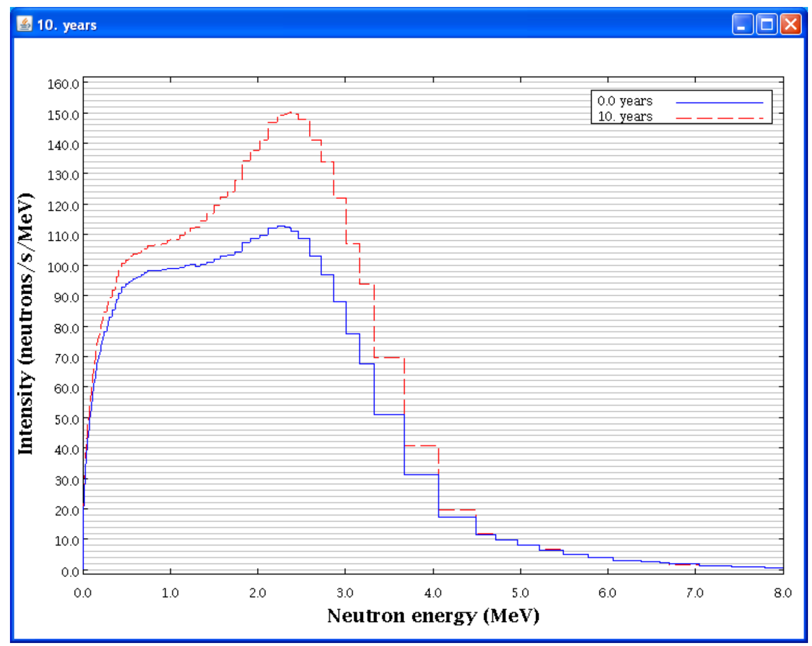
- **Graphical User Input Interface**

MOX input form



- **Java tools for data visualization**

Neutron source spectra (PuO2)



Summary

- ORIGEN is a state-of-the-art burnup and decay analysis code
- Extensively validated and maintained under QA plan
- Next ORIGEN release will contain expanded data/capability
- Monteburns depletion recently upgraded in collaboration with LANL
  - Enhanced capability to use externally supplied cross sections

- Modular ORIGEN package release needed (separate from SCALE)
- Consolidation of development effort needed to support the active up-to-date version of ORIGEN
  - Avoid duplication of effort and parallel development
  - Collaborate on data improvements and new methods development
  - Leverage validation efforts of different organizations
  - Existing experimental database of isotopic data largely underutilized resource for validating nuclear cross section and decay data for fuel cycle R&D (Am, Cm, Cf)
    - ORNL has access to high quality data from International programs

Questions?